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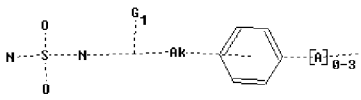

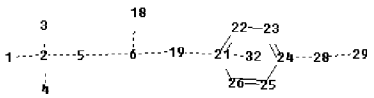

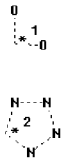

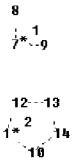

chain nodes :
2 3 4 5 6 7 8 9 18 19 28
ring nodes :
10 11 12 13 14 21 22 23 24 25 26 29
ring/chain nodes :
1
chain bonds :
1-2 2-3 2-4 2-5 5-6 6-18 6-19 7-8 7-9 24-28 28-29
ring bonds :
10-11 10-14 11-12 12-13 13-14 21-26 21-22 22-23 23-24 24-25 25-26
exact/norm bonds :
1-2 2-3 2-4 2-5 5-6 6-18 6-19 7-8 7-9 10-11 10-14 11-12 12-13 13-14
24-28 28-29
normalized bonds :
21-26 21-22 22-23 23-24 24-25 25-26
isolated ring systems :
containing 10 : 21 :

G1:[*1],[*2]

Connectivity :
19:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 18:CLASS 19:CLASS 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 28:CLASS 29:Atom 32:Atom

L1 STRUCTURE UPLOADED

=>
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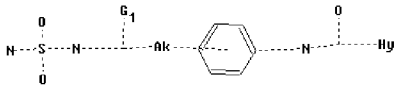

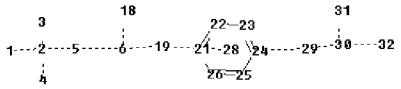

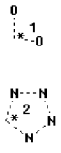

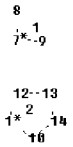

chain nodes :
1 2 3 4 5 6 7 8 9 18 19 29 30 31 32
ring nodes :
10 11 12 13 14 21 22 23 24 25 26
chain bonds :
1-2 2-3 2-4 2-5 5-6 6-18 6-19 7-8 7-9 24-29 29-30 30-31 30-32
ring bonds :
10-11 10-14 11-12 12-13 13-14 21-26 21-22 22-23 23-24 24-25 25-26
exact/norm bonds :
1-2 2-3 2-4 2-5 5-6 6-18 6-19 7-8 7-9 10-11 10-14 11-12 12-13 13-14
24-29 29-30 30-31 30-32
normalized bonds :
21-26 21-22 22-23 23-24 24-25 25-26
isolated ring systems :
containing 10 : 21 :

G1:[*1],[*2]

Connectivity :
19:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 18:CLASS 19:CLASS 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 28:Atom 29:CLASS 30:CLASS 31:CLASS 32:Atom
Generic attributes :
32:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

Element Count :
Node 32: Limited
C,C5
N,N1

L2 STRUCTURE UPLOADED

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=> d his

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L1              STRUCTURE UPLOADED
L2              STRUCTURE UPLOADED
L3           81 S L1 SSS FULL
L4           35 S L2 SSS FULL SUB=L3

     FILE 'CAPLUS' ENTERED AT 16:04:40 ON 11 JUL 2008
L5            2 S L4
L6            2 S US200!-555286/APPS
L7            2 S L5 AND L6
L9            3 S L3
L10           1 S L9 NOT L6


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L7   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2005:1107613  CAPLUS  Full-text
DN   143:326627
TI   Preparation of N-(2-phenylethyl)sulfamide derivatives as α4 integrin
     antagonists for treatment of inflammatory and immune disorders
IN   Jimenez Mayorga, Juan Miguel; Vidal Gispert, Laura; Warrelow, Graham
PA   Almirall Prodesfarma, S.A., Spain
SO   Span., 41 pp.
     CODEN: SPXXAD
DT   Patent
LA   Spanish
FAN.CNT 2
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PI   ES 2219177           A1    20041116    ES 2003-1004           20030505
     ES 2219177           B1    20060216
     WO 2004099126        A1    20041118    WO 2004-EP4670         20040503
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             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
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     EP 1622867           A1    20060208    EP 2004-730833         20040503
     EP 1622867           B1    20070919
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     CN 1816523           A     20060809    CN 2004-80019205       20040503
     JP 2006525271        T     20061109    JP 2006-505356         20040503
     AT 373637            T     20071015    AT 2004-730833         20040503
     ES 2293253           T3    20080316    ES 2004-730833         20040503
     US 20070179183       A1    20070802    US 2006-555286         20061017 <--
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     WO 2004-EP4670       W     20040503
OS   MARPAT 143:326627
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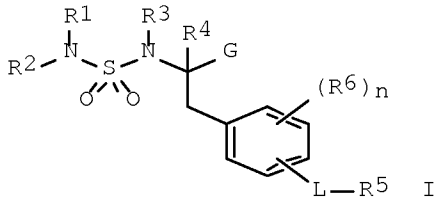

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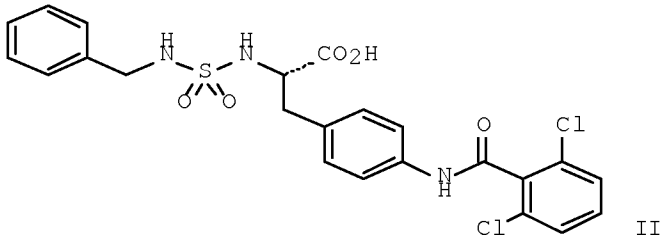

II

AB The invention relates to phenylalanine derivs. I [G = CO2H or tetrazolyl; L = a direct bond, NRc, O, NRcCO, CONRc, O2CNRc, NRcCO2, where Rc = H, alkyl; R1, R2 = independently H, (un)substituted (cyclo)alkyl, alkenyl, alkynyl, heterocyclyl, (hetero)aryl, etc.; or NR1R2 = (un)substituted heterocyclyl, heteroaryl; R3, R4 = H, alkyl; R5 = (un)substituted (hetero)aryl; R6 = OH, alkoxy, NO2, halo, alkylsulfonyl, sulfamoyl, amino, acyl, carboxy, carbamoyl, CN, alkyl, alkenyl, alkynyl, etc.; n = 0-3] and their pharmaceutically-acceptable salts or esters which are α4 integrin antagonists. For example, reaction of Me (2S)-2-[[[(tert- butoxycarbonyl)amino]sulfonyl]amino]-3-[4-[(2,6- dichlorobenzoyl)amino]phenyl]propionate (preparation given) with benzyl alc. in the presence of PBu3 and ADDP in THF, followed by saponification with LiOH•H2O in THF gave (S)-II (43%). In α4β1 adhesion assays, the latter inhibited U-937 cell adhesion to recombinant human soluble VCAM-1 with IC50 values < 100 nM. Thus, I and compns. comprising them are useful for the treatment of inflammatory and immune disorders (no data).

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:996111 CAPLUS Full-text
DN 141:410709
TI Preparation of N-(2-phenylethyl)sulfamide derivatives as integrin α4 antagonists for treatment of inflammatory and immune disorders
IN Jimenez Mayorga, Juan Miguel; Vidal Gispert, Laura; Warrellow, Graham
PA Almirall Prodesfarma, S.A., Spain
SO PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004099126	A1	20041118	WO 2004-EP4670	20040503

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LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
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SN, TD, TG

ES	2219177	A1	20041116	ES 2003-1004	20030505
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EP	1622867	A1	20060208	EP 2004-730833	20040503
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

CN	1816523	A	20060809	CN 2004-80019205	20040503
JP	2006525271	T	20061109	JP 2006-505356	20040503
US	20070179183	A1	20070802	US 2006-555286	20061017 <--
PRAI ES	2003-1004	A	20030505		
	WO 2004-EP4670	W	20040503		

OS MARPAT 141:410709

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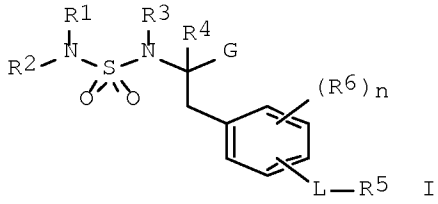

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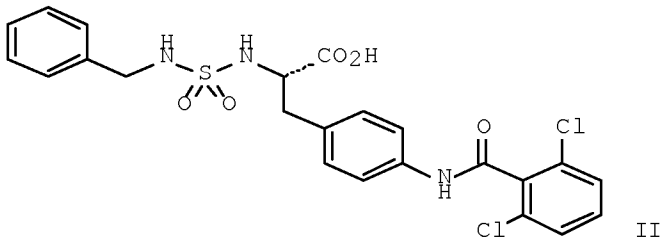

II

AB Title compds. L-phenylalanine derivs. I [wherein G = CO2H, tetrazolyl; L = direct bond, NRc, O, NRcCO, CONRc, OCONRc, NRcCO2; Rc = H, alkyl; R1, R2 = independently H, (un)substituted (cyclo)alkyl, alkenyl, alkynyl, heterocyclyl, (hetero)aryl, etc.; or NR1R2 = (un)substituted heterocyclyl, heteroaryl; R3, R4 = H, alkyl; R5 = (un)substituted (hetero)aryl; R6 = OH, alkoxy, NO2, halo, alkylsulfonyl, sulfamoyl, amino, acyl, carboxy, carbamoyl, CN, alkyl, alkenyl, alkynyl, etc.; n = 0-3; and pharmaceutically acceptable salts and esters thereof] were prepared as integrin α4 antagonists. For example, reaction of Me (2S)-2-[[[(tert-butoxycarbonyl)amino]sulfonyl]amino]-3-[4-[(2,6-dichlorobenzoyl)amino]phenyl]propionate (preparation given) with benzyl alc. in the presence of PBu3 and ADDP in THF, followed by saponification with LiOH•H2O in THF gave (S)-II (43%). In α4β1 adhesion assays, the latter inhibited U-937 cell adhesion to recombinant human soluble VCAM-1 with IC50

values < 100 nM. Thus, I and compns. comprising them are useful for the treatment of inflammatory and immune disorders (no data).

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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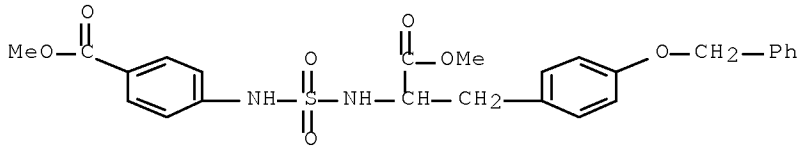
L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2000:41769 CAPLUS Full-text
DN 132:194332
TI Synthesis of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives and evaluation of their affinity for MHC class-II proteins
AU Ducry, Laurent; Reinelt, Stefan; Seiler, Paul; Diederich, Francois; Bolin, David R.; Campbell, Robert M.; Olson, Gary L.
CS Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule, ETH-Zentrum, Zurich, CH-8092, Switz.
SO Helvetica Chimica Acta (1999), 82(12), 2432-2447
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
AB 1,2,5-Thiadiazolidin-3-one 1,1-dioxide derivs. were designed by mol. modeling as MHC (major histocompatibility complex) class-II inhibitors. They were prepared from the unsym. N,N'-disubstituted acyclic sulfamides. These N-alkyl-N'-arylsulfamide precursors were synthesized by nucleophilic substitution of either a sulfamoyl chloride or a N-sulfamoyloxazolidinone. Extension of base-induced cyclization methods from aliphatic to aromatic sulfamides gave access to the desired target mols. The N-alkyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide derivs. were also prepared by the oxazolidinone route for coupling to a tetrapeptide fragment. The X-ray crystal structure of 1,2,5-thiadiazolidin-3-one 1,1-dioxide was solved, and the directionality of the H-bond donor (N-H) and acceptor (SO2) groups of the cyclic scaffold determined 1,2,5-Thiadiazolidin-3-one 1,1-dioxides were shown to inhibit competition peptide binding to HLA-DR4 mols. in the single-digit millimolar concentration range.
IT 259794-36-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiadiazolidinone dioxide derivs. and evaluation of their affinity for MHC class-II proteins)
RN 259794-36-0 CAPLUS
CN Tyrosine, N-[[[4-(methoxycarbonyl)phenyl]amino]sulfonyl]-O-(phenylmethyl)-, methyl ester (CA INDEX NAME)



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STN INTERNATIONAL SESSION SUSPENDED AT 16:06:13 ON 11 JUL 2008